10/656974

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=> d his

     (FILE 'HOME' ENTERED AT 10:19:20 ON 07 FEB 2005)

     FILE 'REGISTRY' ENTERED AT 10:28:38 ON 07 FEB 2005
L1                STR
L2                STR L1
L3             0 S L2
L4                STR L2
L5             0 S L4
L6                STR L4
L7             0 S L6
L8             0 S L7 FUL

     FILE 'BEILSTEIN' ENTERED AT 10:56:25 ON 07 FEB 2005
L9             0 S L6 FUL

     FILE 'REGISTRY' ENTERED AT 11:03:31 ON 07 FEB 2005
L10               STR L6
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L12               STR L11
L13            0 S L12
L14            4 S L12 FUL

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L12 HAS NO ANSWERS
L12               STR
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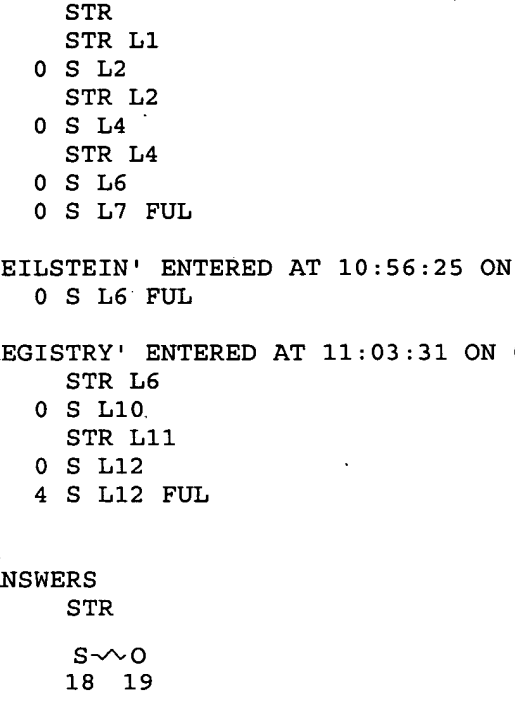


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REP G1=(1-5) CH2
NODE ATTRIBUTES:
HCOUNT   IS E2      AT   1
HCOUNT   IS E2      AT   4
HCOUNT   IS E2      AT  12
HCOUNT   IS E2      AT  13
HCOUNT   IS E2      AT  14
HCOUNT   IS E2      AT  15
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  14

STEREO ATTRIBUTES: NONE

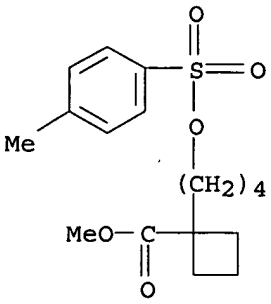

=> d l14 3 all

L14  ANSWER 3 OF 4  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   69873-99-0  REGISTRY
```

ED Entered STN: 16 Nov 1984
CN Cyclobutanecarboxylic acid, 1-[4-[[(4-methylphenyl)sulfonyl]oxy]butyl]-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H24 O5 S
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C4	C4	4	C4	4.209.1	1
C6	C6	6	C6	46.150.18	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	175	pH 1	(1) ACD
Bioconc. Factor (BCF)	175	pH 4	(1) ACD
Bioconc. Factor (BCF)	175	pH 7	(1) ACD
Bioconc. Factor (BCF)	175	pH 8	(1) ACD
Bioconc. Factor (BCF)	175	pH 10	(1) ACD
Boiling Point (BP)	450.9+/-18.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	70.98+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	226.5+/-38.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	9		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1404	pH 1	(1) ACD
Koc (KOC)	1404	pH 4	(1) ACD
Koc (KOC)	1404	pH 7	(1) ACD
Koc (KOC)	1404	pH 8	(1) ACD
Koc (KOC)	1404	pH 10	(1) ACD
logD (LOGD)	3.25	pH 1	(1) ACD
logD (LOGD)	3.25	pH 4	(1) ACD
logD (LOGD)	3.25	pH 7	(1) ACD
logD (LOGD)	3.25	pH 8	(1) ACD

logD (LOGD)	3.25	pH 10	(1) ACD
logP (LOGP)	3.255+/-0.626		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	340.44		(1) ACD
Vapor Pressure (VP)	2.55E-08 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 90:186469 CA
TI Prostaglandin analogs
IN Kurono, Masayasu; Hamanaka, Nobuyuki; Sakuyama, Shigeru; Chiba, Takeshi; Nakai, Hisao
PA Ono Pharmaceutical Co., Ltd., Japan
SO Ger. Offen., 71 pp.
CODEN: GWXXBX
DT Patent
LA German
IC C07C177-00
CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 63

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2830478	A1	19790201	DE 1978-2830478	19780711
	DE 2830478	C2	19851024		
	JP 54019946	A2	19790215	JP 1977-83558	19770714
	JP 60022708	B4	19850603		
	FR 2397402	A1	19790209	FR 1978-20818	19780712
	FR 2397402	B1	19830624		
	GB 2002355	A	19790221	GB 1978-29756	19780713
	GB 2002355	B2	19820421		
	US 4208428	A	19800617	US 1978-924343	19780713
PRAI	JP 1977-83558	19770714			

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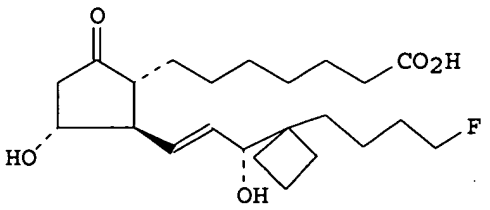

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AB Prostaglandin F and F analogs of the 1 and 2 series containing a cyclobutane ring in the ω-chain and a halogen atom in the ω-position were prepared by appropriate modifications of the phosphonic acid used to introduce the ω-chain in conventional syntheses. Thus prepared were

.apprx.35 such prostaglandins (e.g., I) and intermediates for them.

ST prostaglandin omega cyclobutyl halo

IT Prostaglandins
RL: RCT (Reactant); RACT (Reactant or reagent)
(analogs, ω-cyclobutyl-ω-halo)

IT 3721-95-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of, with (4-chlorobutoxy)tetrahydropyran)

IT 31752-99-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)

IT 41302-05-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and alkylation of cyclobutanecarboxylic acid with)

IT 69873-87-6P 69874-03-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and borohydride reduction of)

IT 69873-91-2P 69874-08-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)

IT 69873-83-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and esterification-partial hydrolysis of)

IT 69873-89-8P 69874-06-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydride reduction of)

IT 69873-93-4P 69874-10-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

IT 69873-92-3P 69874-09-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and partial hydrogenation of)

IT 69873-88-7P 69873-94-5P 69874-11-9P 70095-05-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and partial hydrolysis of)

IT 69873-84-3P 69874-05-1P 69896-51-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and protection with dihydropyran)

IT 69873-90-1P 69874-07-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with (4-carboxybutyl)triphenylphosphonium bromide)

IT 69873-85-4P 69874-01-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with di-Me methylphosphonate)

IT 69873-99-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with lithium bromide)

IT 69873-96-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with lithium halides)

IT 69874-00-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with sodium fluoride-sulfur tetrafluoride)

IT 69873-95-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and tosylation of)
IT 38754-71-1P 69873-86-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and use in prostaglandin syntheses)
IT 69874-02-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and use in prostaglandin synthesis)
IT 69873-97-8P 69873-98-9P 69874-04-0P 69874-12-0P 69926-70-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 928-51-8
RL: PROC (Process)
(protection of, with dihydropyran)
IT 17814-85-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(use of, in synthesis of cyclobutyl analogs of prostaglandins)
IT 756-79-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(use of, in synthesis of cyclobutylprostaglandin analogs)

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pairs were found to correlate between the enzyme forms with a slope of 1.03, suggesting that the hemopexin domain does not significantly modify the enzyme active-site structure.

L13 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
2003:977318 Document No. 140:195327 The Intermediate S1' Pocket of the Endometase/Matrilysin-2 Active Site Revealed by Enzyme Inhibition Kinetic Studies, Protein Sequence Analyses, and Homology Modeling. Park, Hyun I.; Jin, Yonghao; Hurst, Douglas R.; Monroe, Cyrus A.; Lee, Seakwoo; Schwartz, Martin A.; Sang, Qing-Xiang Amy (Department of Chemistry and Biochemistry and Institute of Molecular Biophysics, Florida State University, Tallahassee, FL, 32306-4390, USA). Journal of Biological Chemistry, 278(51), 51646-51653 (English) 2003. CODEN: JBCHA3. ISSN: 0021-9258. Publisher: American Society for Biochemistry and Molecular Biology.
AB Human matrix metalloproteinase-26 (MMP-26/endometase/matrilysin-2) is a newly identified MMP and its structure has not been reported. The enzyme active site S1' pocket in MMPs is a well-defined substrate P1' amino acid residue-binding site with variable depth. To explore MMP-26 active site structure-activity, a series of new potent mercaptosulfide MMP inhibitors (MMPIs) with Leu or homophenylalanine (Homophe) side chains at the P1' site were selected. The Homephe side chain is designed to probe deep S1' pocket MMPs. These inhibitors were tested against MMP-26 and several MMPs with known x-ray crystal structures to distinguish shallow, intermediate, and deep S1' pocket characteristics. MMP-26 has an inhibition profile most similar to those of MMPs with intermediate S1' pockets. Investigations with hydroxamate MMPIs, including those designed for deep pocket MMPs, also indicated the presence of an intermediate pocket. Protein sequence anal. and homol. modeling further verified that MMP-26 has an intermediate S1' pocket formed by Leu-204, His-208, and Tyr-230. Moreover, residue 233 may influence the depth of an MMP S1' pocket. The residue at the equivalent position of MMP-26 residue 233 is hydrophilic in intermediate-pocket MMPs (e.g., MMP-2, -8, and -9) and hydrophobic in deep-pocket MMPs (e.g., MMP-3, -12, and -14). MMP-26 contains a His-233 that renders the S1' pocket to an intermediate size. This study suggests that MMPIs, protein sequence analyses, and mol. modeling are useful tools to understand structure-activity relationships and provides new insight for rational inhibitor design that may distinguish MMPs with deep vs. intermediate S1' pockets.

L13 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
2002:818382 Document No. 138:187590 A practical synthesis of differentially-protected cis-1,2-cyclopentanedithiols and cis-3,4-pyrrolidinedithiols. Jin, Yonghao; Ghaffari, Mohammad A.; Schwartz, Martin A. (Department of Chemistry and Biochemistry, The Florida State University, Tallahassee, FL, 32306, USA). Tetrahedron Letters, 43(41), 7319-7321 (English) 2002. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 138:187590. Publisher: Elsevier Science Ltd..
AB A practical method for the synthesis of cis-1,2-cyclopentanedithiols and cis-3,4-pyrrolidinedithiols with differentially protected sulfurs, needed for the design of new metal-chelating ligands, has been developed.

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(FILE 'HOME' ENTERED AT 14:16:37 ON 03 FEB 2005)

FILE 'REGISTRY' ENTERED AT 14:16:48 ON 03 FEB 2005
L1 STR
L2 20 S L1
L3 STR
L4 50 S L3
L5 STR L3
L6 10 S L5
L7 STR